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Predictive Modeling of the CDRA Four Bed Molecular Sieve

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Introduction

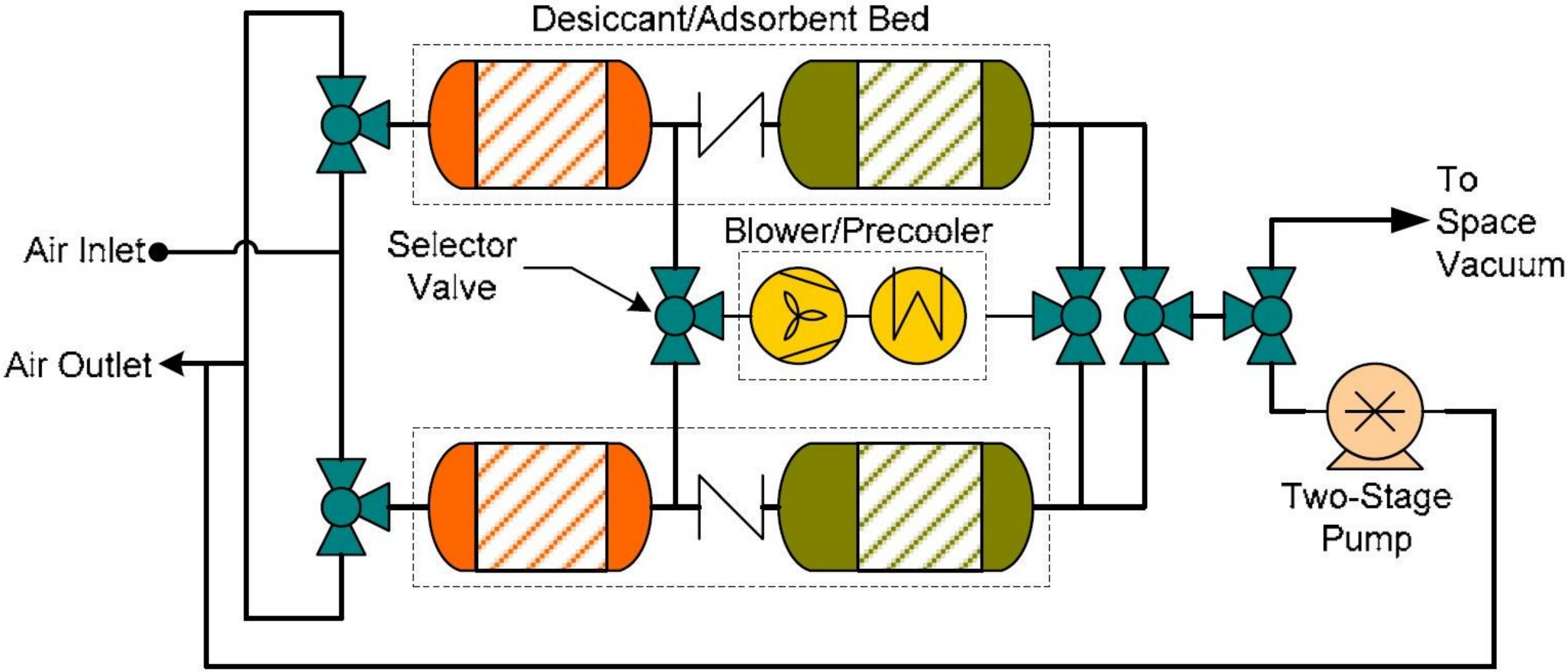
- Advanced Exploration Systems (AES) Program
  - the Life Support Systems Project (LSSP)

- Rapid development of prototype systems
- Concept validation for human missions beyond LEO
- Reduce developmental and mission risk
- Derived from ISS subsystem architecture

➢ Virtual Laboratory via Simulation

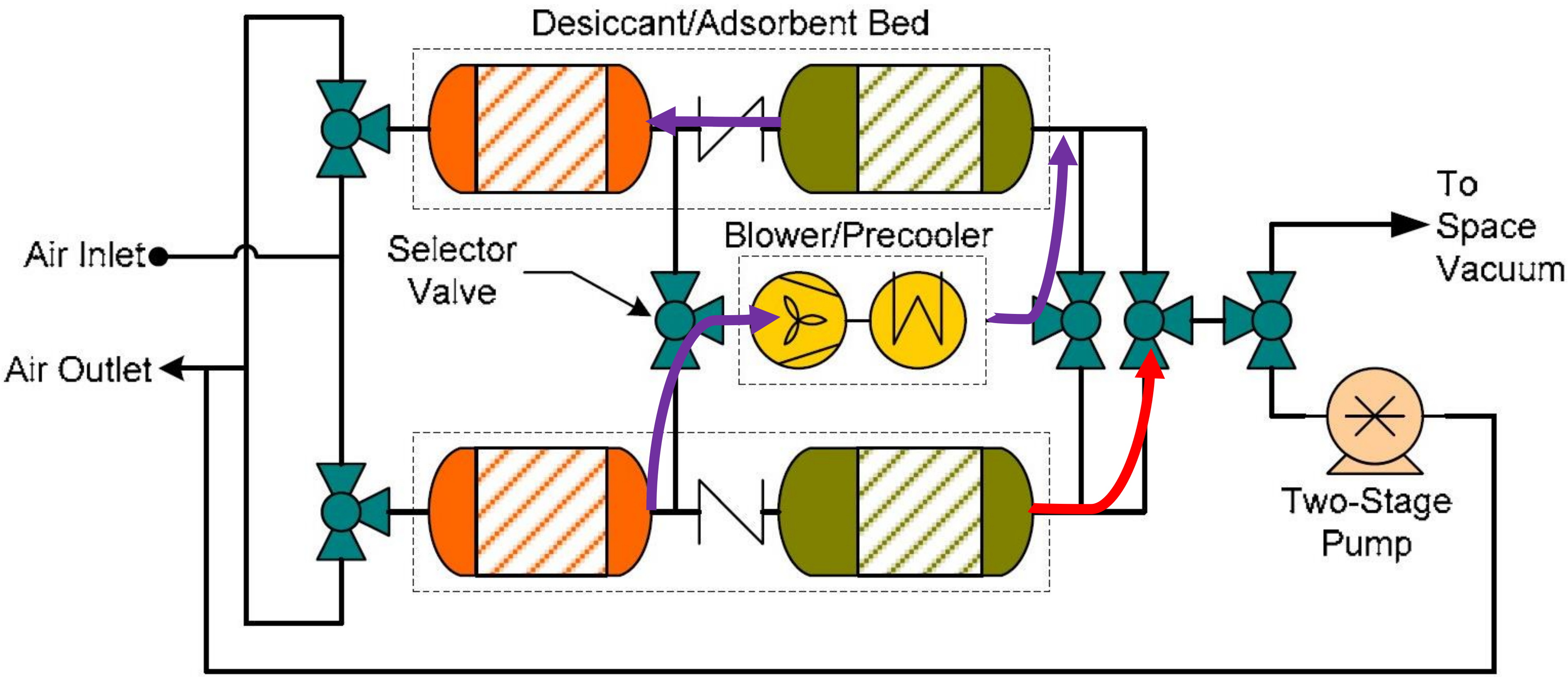
Carbon Dioxide Removal Assembly (CDRA)

- We are now predictively modeling the entire four Bed Molecular Sieve (4BMS)
  - CO_2 removal rate, efficiency, effluent dew point, power
- No Sabatier included (yet)
- Temperature details still need work…



CDRA version 4 Engineering Unit (CDRA-4EU)

- Every ‘half-cycle’ the system switches flow directions
- Desorbing sorbent bed is heated & evacuated (red)
- Desiccant beds (orange) remove and return H_2O
- Adsorbent beds (green) remove CO_2



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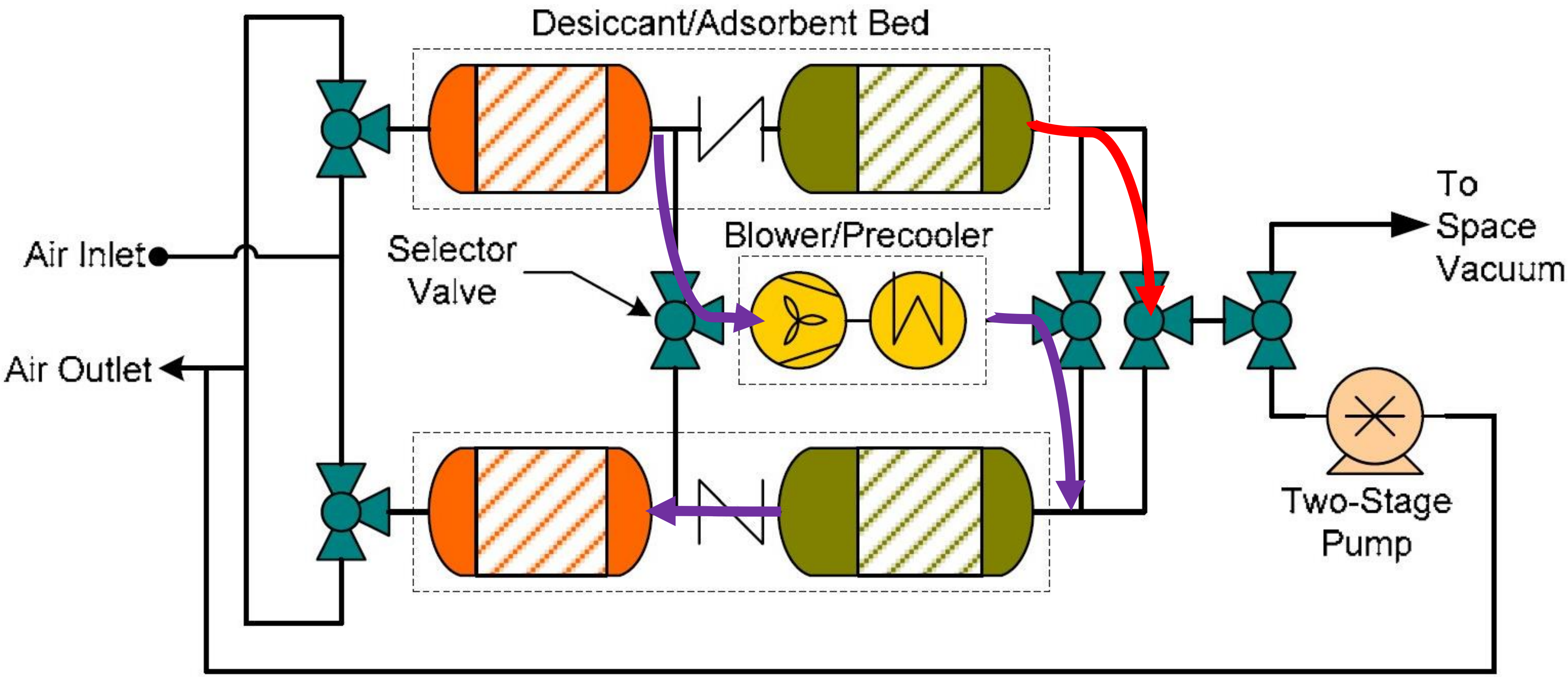
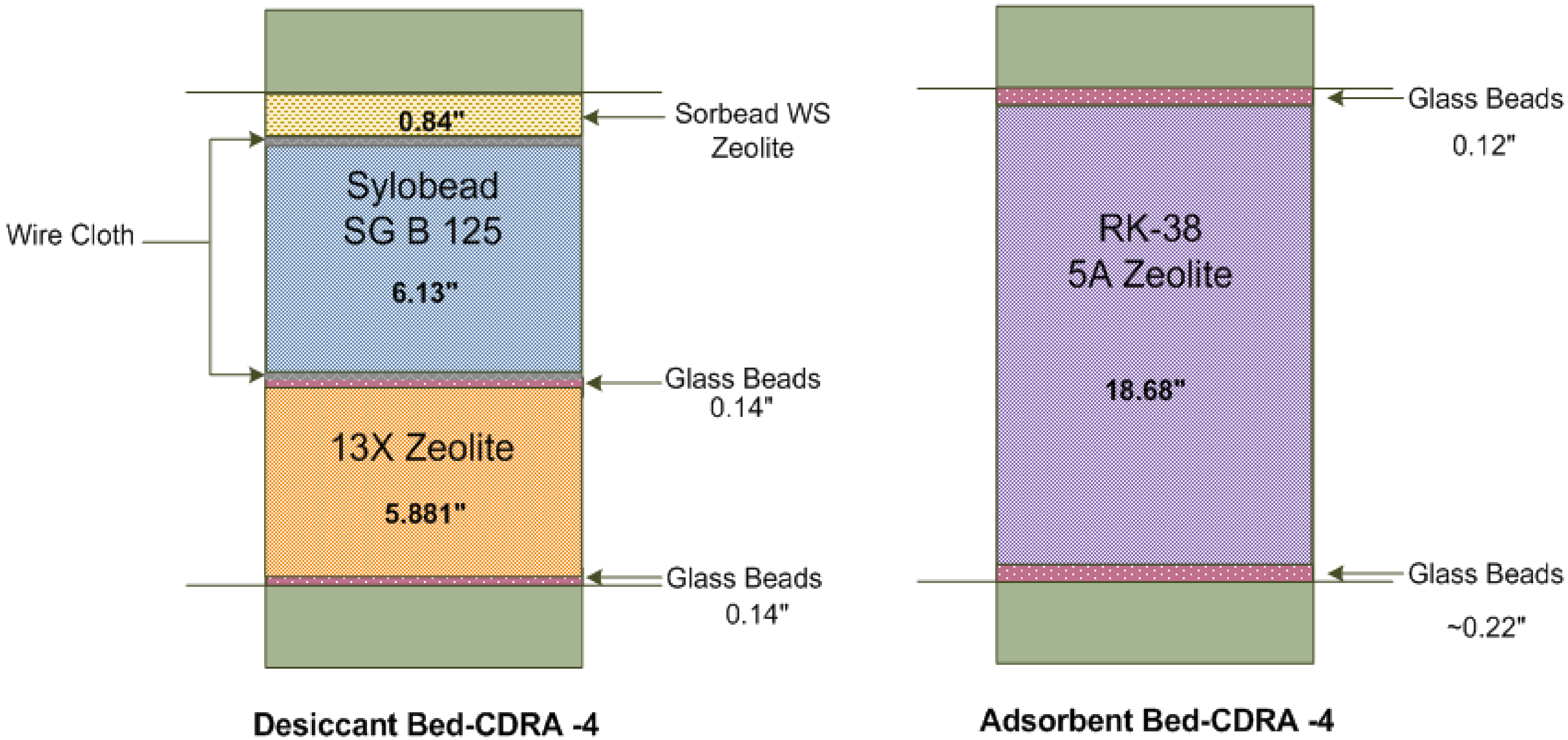
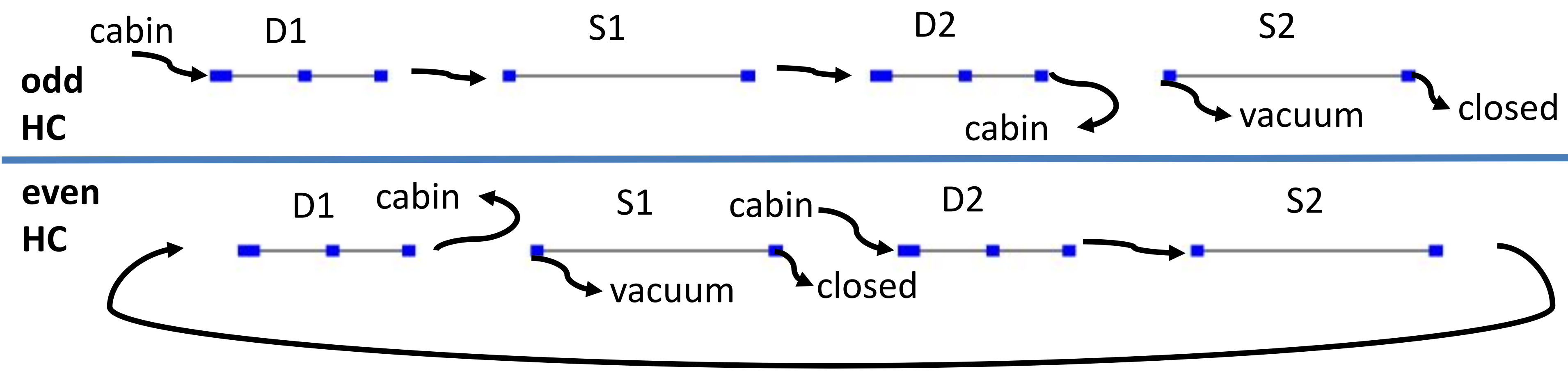


CDRA-4EU Four Beds



- Two of each bed
- Glass bead layers treated as inactive to H_2O and CO_2
- Wire cloths not modeled
- Aluminum can and insulation included in model
- Beds are square in cross-section

CDRA-4EU 4BMS 1-D COMSOL Model



- Changes boundary conditions every half-cycle
- Separate thermal solutions for sorbent, gas, can, insulation
- Sorbate mass fraction effluent values are influent conditions for next bed
- Each container solved separately
- Sorbent bed desorbed via vacuum and internal heating

Model Details

- Uses dimensionless correlations (Re, Nu, Pe, Pr, Sc)
- Some simplifying assumptions such as:
  - Darcy flow
  - binary mass diffusion
  - constant porosity
  - Rumpf-Gupte permeability
  - 1D ‘plug flow’ style model with wall corrections
  - simple isotherms
- Use other tests to calibrate LDF, heat transfer, and porosity
- Use COMSOL Multiphysics modules to solve the flow, transport, and thermal PDEs

CDRA-4EU Application

- Explored parameter space:
  - 75 to 215 min half-cycles (limited by heater)
  - 20 to 34 SCFM flow rates (limited by blower)
- Nominal operating conditions
  - 10 minute air-save mode on desorbing sorbent bed
  - Single P(t) desorption profile
  - 53 degF inlet temp
  - 50 degF inlet dew point
  - 70 degF ambient temp
  - 2 torr inlet CO_2 partial pressure

Comparison to CDRA-4EU Data

HC	flow rate	CO2 removal rate (kg/day)			efficiency		
(min)	(SCFM)	data	model	delta %	data	model	delta %
155	20.4	3.65	3.35	8.2	0.843	0.789	6.4
90	25.0	4.11	3.73	9.2	0.772	0.716	7.3
90	24.0	3.76	3.70	1.6	0.745	0.696	6.6
215	20.0	3.18	3.12	1.9	0.779	0.749	3.9
172	25.0	4.05	3.90	3.7	0.783	0.749	4.3
144	30.0	4.83	4.62	4.3	0.740	0.740	0.0
123	34.0	5.18	5.44	-5.0	0.712	0.769	-8.0
195	20.0	3.49	3.41	2.3	0.813	0.818	-0.6
154	25.0	4.19	4.30	-2.6	0.812	0.826	-1.7
124	30.0	5.14	5.18	-0.8	0.781	0.830	-6.3
96	34.0	5.69	5.82	-2.3	0.810	0.822	-1.5

- *All cases match removal rate and efficiency to better than 10%*
- Test inputs (dew point, inlet temperature, ambient temperature, heater power, flow rate) vary from test to test and within a test
- Expected model uncertainty ~10%, so Virtual Laboratory is ready!

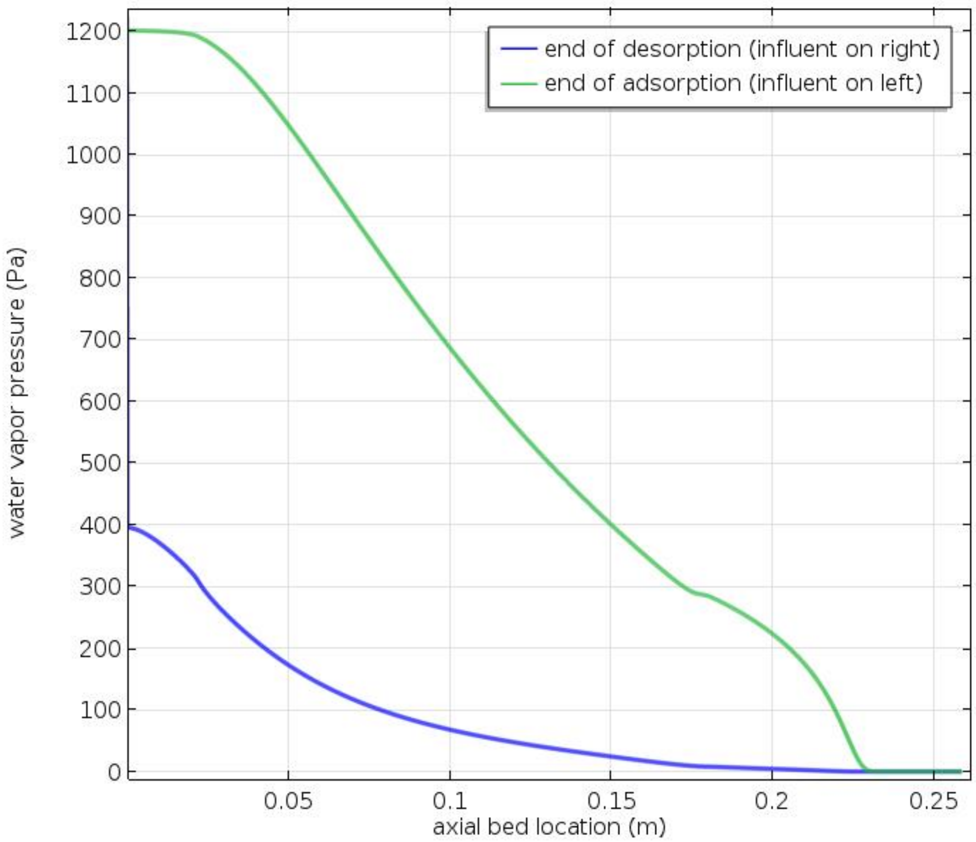
Observations from the Model

- Bed to bed variation (e.g. heaters) can be large
- In old nominal operation (20/155/4), CO_2 nearly fills sorbent bed (“flat-line”)
- 13X sorbent is serving as a CO_2 ‘reservoir’
- Heaters are not fully effective (heat leak)
- Temperature profiles not well matched (1-D limit)
- Significant H_2O margin in the 13X layer
  - System robust to contamination due to e.g. siloxanes

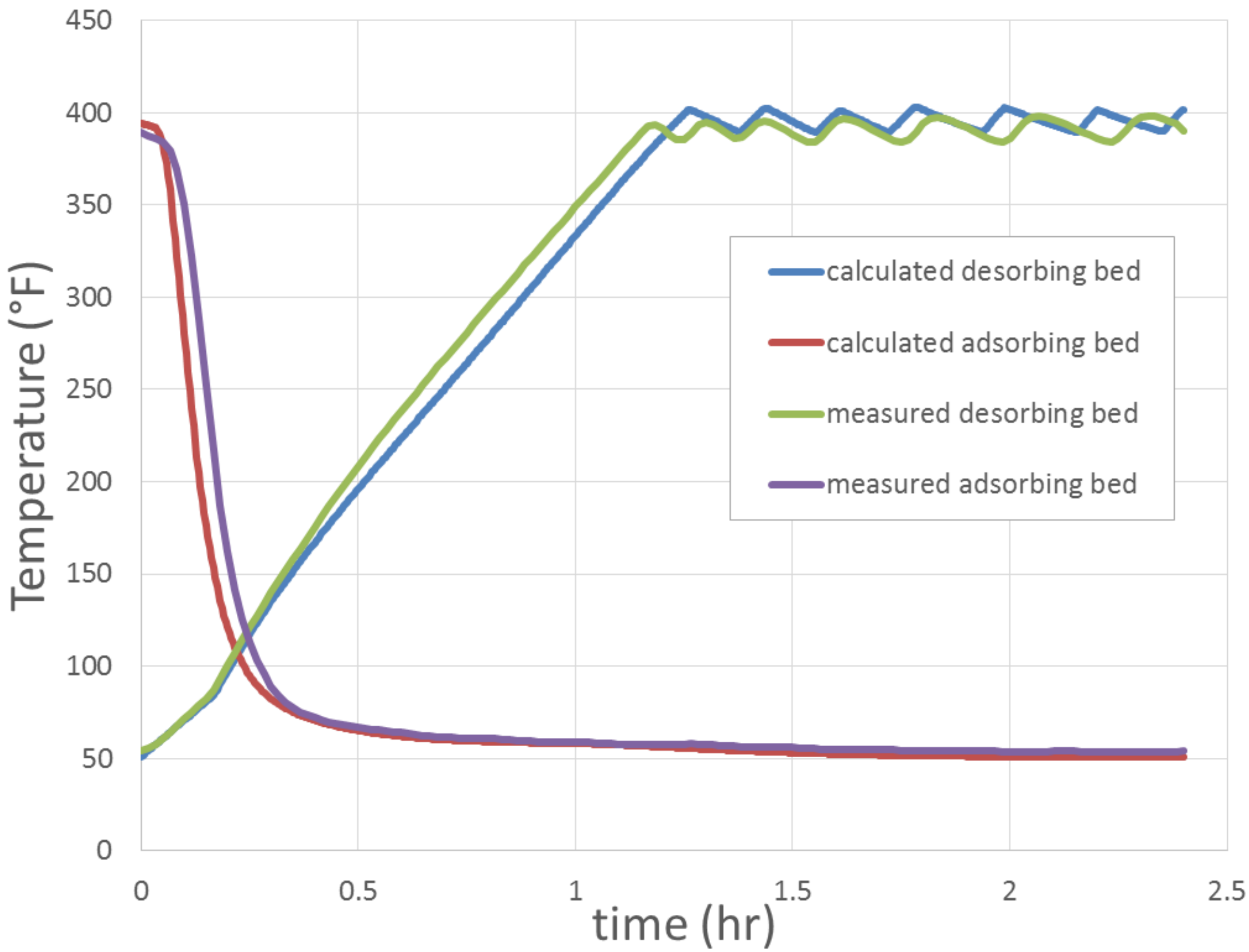
4BMS for Exploration (4BMS-X)

– If 13X has H_2O margin and is a CO_2 reservoir, can we remove it?
  - Save mass and volume and improve efficiency

- Optimized models show 28 SCFM and 80 min HC will meet the 4BMS-X 4.16 kg/day CO_2 removal rate with half of the 13X layer removed
- More 13X can be removed with lower inlet dew point



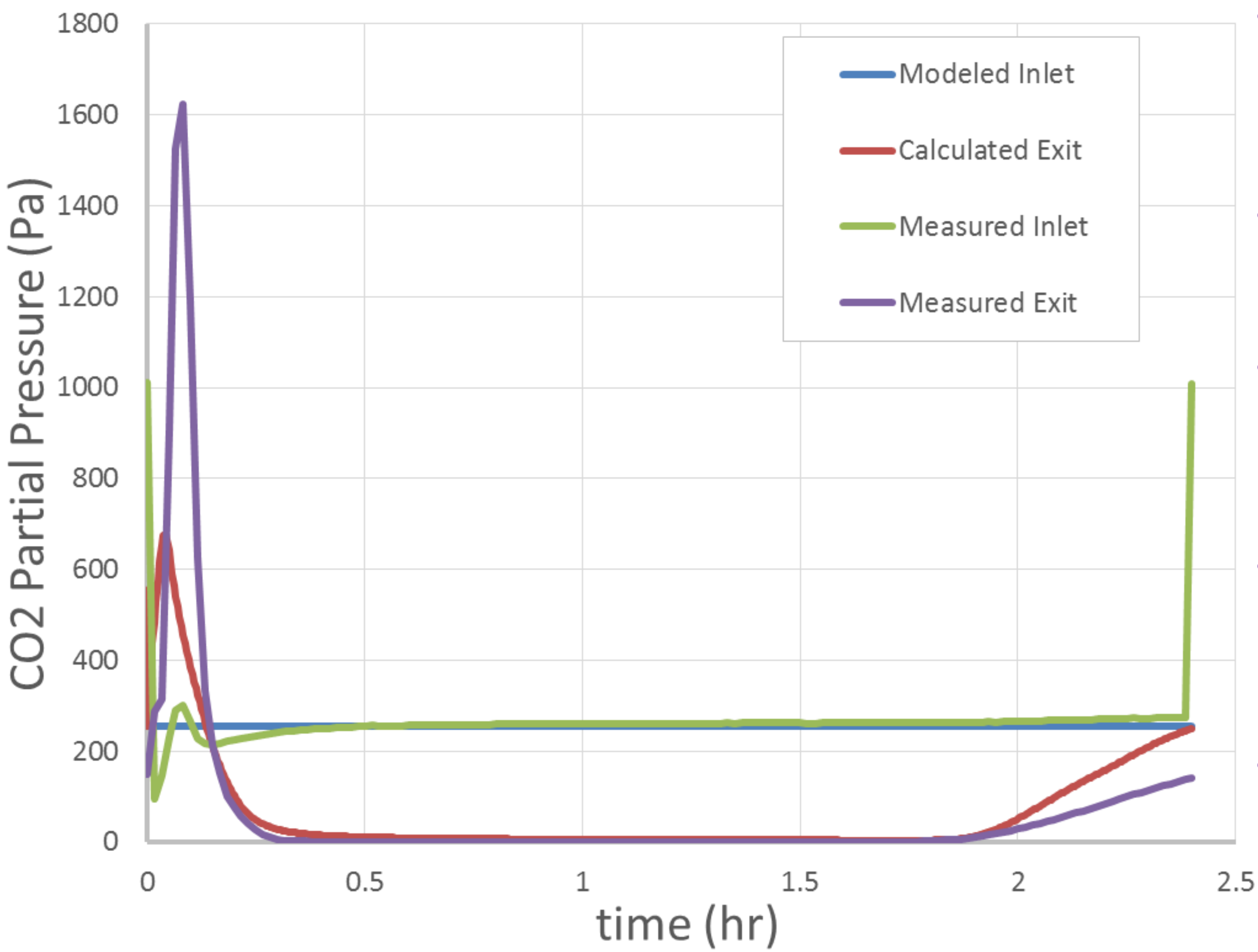
Temperature Results



- Data shows variations not captured in simulation
- Heating and cooling balance not perfect
- Performance impact minimal

Representative (30/144/2) comparison of temperature at the CDRA-4EU heater controlling RTD location

CO_2 Partial Pressure Results



- Data shows variation in inlet CO_2 not captured in simulation
- CO_2/H_2O competition on 13X poorly known
- 5A Toth isotherm probably inaccurate at low loading
- Model predicts CO_2 'flat-line' and start of H_2O breakthrough
- Model plot does not include air-save component

Representative (30/144/2) comparison of CO_2 partial pressure into and out of the CDRA-4EU

Summary

- Predictive COMSOL model of CDRA-like system
- Can change all model inputs in the simulation:
  - Bed size, layer size, sorbent, temperatures, heaters, geometry, can, insulation, everything!
- Limit of data stability and uncertainty being reached
- 1-D model limitations are being reached
  - Radial heat flow
  - Channeling effects

➢ Virtual Laboratory helping design next generation CDRA for Exploration